

4-Bromo-5-methoxy-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)thiophene-2-carboxamide
113589-05-2 | DTXSID60556730

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.12e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.74e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Benomyl</div> <div>Measured: 1.31e-05</div> <div>Predicted: 3.43e-03</div>	<div>Image not found</div> <div>Methidathion</div> <div>Measured: 6.19e-04</div> <div>Predicted: 1.05e-03</div>	<div>Image not found</div> <div>Azinphos-methyl</div> <div>Measured: 6.59e-05</div> <div>Predicted: 5.36e-04</div>
<div>Image not found</div> <div>2,4-Bis((3-methoxypropyl)amino)-6(methylthio)-s-triazine</div> <div>Measured: 3.32e-04</div> <div>Predicted: 1.23e-02</div>	<div>Image not found</div> <div>Azinphos-ethyl</div> <div>Measured: 3.04e-05</div> <div>Predicted: 1.88e-04</div>	